403 Poyntz Avenue, Suite B
Manhattan, KS 66502
USA
+1.785.770.8511
www.thunderheadeng.com

TOUGH2/T2VOC Examples

PetraSim 5

TOUGH2/T2VOC Examples

Table of Contents

Disclaimer viii
Acknowledgements ix
1. Five-Spot Geothermal Injection and Production 1
Create a New Model 1
Edit Layers 1
Create Mesh 2
Edit Global Properties 2
Edit Materials 2
Initial Conditions 3
Edit Injection and Production Cells 3
Edit Solution Controls 4
Edit Output Controls 4
Save and Run 4
View 3D Results 5
View Time History Plots 6
2. Production from a Geothermal Reservoir (EWASG) 8
Description 8
Create an EWASG Model 8
Specify the Solution Mesh 8
Specify Z Divisions 8
Create the Mesh 9
Global Properties 9
Material Properties 10
Initial Conditions 11
Define Reservoir Production 11
Solution Controls 12
Output Controls 12
Save and Run 12
View 3D Results 13
View Cell History Plots 14
Line Plots 15
3. 2D Steam Replacement (T2VOC) 17
Description 17
Create a T2VOC Model 17
Specify the Solution Mesh 18
Specify Z Divisions 18
Create the Mesh 18
Global Properties 19
Simulation Name 19
EOS Data 19
Material Properties 20
Initial Conditions 21
Boundary Conditions 22
Solution Controls 23
Output Controls 23

Save and Run.....23
View 3D Results.....24
References.....26

Figures

Figure 1.1: Diagram of reservoir for Five-Spot Injection 1
Figure 1.2: The Running TOUGH2 dialog shows a graph of time step size. 5
Figure 1.3: Temperature contours at end of solution 6
Figure 1.4: Temperature history of injection cell. 7
Figure 2.1: The resulting model 9
Figure 2.2: The cell to be selected 12
Figure 2.3: 3D representation of the saturation of gas 14
Figure 2.4: The cell history plot for gas saturation in the production cell 15
Figure 2.5: Line plot of pressure 16
Figure 2.6: Results for comparison with TOUGH2 manual 16
Figure 3.1: Example Problem Overview 17
Figure 3.2: The Model Boundary 18
Figure 3.3: T2VOC Simulation Parameters 20
Figure 3.4: Finding a Cell in the 3D View 22
Figure 3.5: Running T2VOC 24
Figure 3.6: T2VOC 3D Results 25

List of Tables

Table 2.1: Model boundary dimensions 8
Table 3.1: Model boundary dimensions 17
Table 3.2: Chlorobenzene Ex 1 (CHEMP.4) 19
Table 3.3: Chlorobenzene Ex 1 (CHEMP.6) 20
Table 3.4: Chlorobenzene Ex 1 (CHEMP.7) 20

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Users are warned that PetraSim is intended for use only by those competent in the field of multi-phase, multi-component fluid flow in porous and fractured media. PetraSim is intended only to supplement the informed judgment of the qualified user. The software package is a computer model that may or may not have predictive capability when applied to a specific set of factual circumstances. Lack of accurate predictions by the model could lead to erroneous conclusions. All results should be evaluated by an informed user.

Throughout this document, the mention of computer hardware or commercial software does not constitute endorsement by Thunderhead Engineering, nor does it indicate that the products are necessarily those best suited for the intended purpose.

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In preparing this manual, we have liberally used descriptions from the user manuals for the TOUGH family of codes. Links to download the TOUGH manuals are given at http://www.petrasim.com. More information about the TOUGH family of codes can be found at: http://www-esd.lbl.gov/TOUGH2/. Printed copies of the user manuals may be obtained from Karsten Pruess at <K_Pruess@lbl.gov>.

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We most sincerely thank our users for their feedback and support.

1. Five-Spot Geothermal Injection and Production

This example is *Problem 4 - Five Spot Geothermal Production and Injection (EOS1, EOS2)* described in the TOUGH2 User's Manual (1). This example simulates a five-spot pattern of injection and production from a geothermal reservoir. Only one quarter of the reservoir is included, since the solution is symmetric, as shown in Figure 1.1. The mesh uses cells of uniform 50 m x 50 m size.

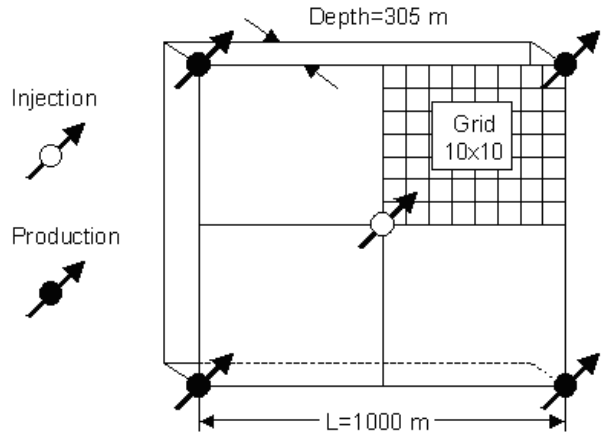

Figure 1.1: Diagram of reservoir for Five-Spot Injection

We will solve this example using a porous media assumption for the formation.

Create a New Model

This example will use EOS1, the equation of state module that models multi-phase water and tracer. The dimensions of the model will be 500x500x305 meters. This information can be entered using the **New** dialog.

To create the model:

1. On the **File** menu, click **New**
2. In the **Simulator Mode** list, select **TOUGH2**
3. In the **Equation of State (EOS)** list, select **EOS1**
4. In the **X Max** box, type *500*
5. In the **Y Max** box, type *500*
6. In the **Z Max** box, type *305*
7. Click **OK** to close the dialog and create the model

Edit Layers

Before creating the mesh, we must first define the model layers. Layers in PetraSim define depth-based boundaries that can provide a convenient way to manage multiple rock layers. When the mesh is generated, the layer boundary will become the boundary between cells and each layer can be divided into an arbitrary number of internal divisions – these internal divisions will also become cell boundaries.

By default, the model is created with a single layer. Because this example contains only a single cell in the Z-direction, the layer must be edited to contain only a single cell.

To set the default layer to use a single vertical cell:

1. In the Tree View, expand the **Layers** node and click **Default**
2. On the **Edit** menu, click **Properties...**
3. In the **Cells** box, type *1*
4. Click **OK** to save changes to the default layer

Create Mesh

To create a 10 x 10 regular mesh:

1. On the **Model** menu, click **Create Mesh**
2. In the **X Cells** box, type *10*
3. In the **Y Cells** box, type *10*
1. Click **OK** to create the mesh

Edit Global Properties

Global properties apply to the entire model. In this example, the only item to change is the analysis name. To set the simulation name:

1. On the **Properties** menu, click **Global Properties**
2. In the **Name** box, type *Five Spot Production and Injection*
3. Click **OK**

Edit Materials

This simulation will require only one material. To specify material properties:

1. On the **Properties** menu, click **Edit Materials...**
2. In the **Name** box, type *POMED*
3. In the **Density** box, type *2650.0*
4. In the **Porosity** box, type *0.01*
5. In all three **Permeability** boxes (X, Y, and Z), type *6e-15*

For this simulation we will define relative permeability using Corey's Curves. To specify the relative permeability for this material:

1. Click **Additional Material Data...**
2. In the **Relative Permeability** list, click **Corey's Curves**
3. Click **OK**

Click **OK** to save changes and exit the **Edit Materials** dialog.

Initial Conditions

When specifying parameters such as initial conditions, PetraSim uses a tiered system that allows cells to inherit values from the containing region, regions from the containing layer, and layers from the global defaults. Once we set the default initial conditions, these values will be used by all cells except those where we have explicitly set values.

Correct specification of initial conditions is essential for simulation convergence. The initial conditions must be physically meaningful. Often this requires an initial state analysis in which a model is run to obtain initial equilibrium conditions before the analysis of interest (geothermal production, VOC spill, etc.) is run.

However, in 2D models with no pressure gradient (such as this) this process is simplified somewhat.

To set the global initial conditions:

1. On the **Properties** menu, click **Initial Conditions...**
2. In the **EOS1** list, select **Two-Phase (T, Sg)**
3. In the **Temperature** box, type *300*
4. In the **Gas Saturation** box, type *0.01*
5. Click **OK** to save changes and exit the dialog

Selecting a two-phase initial state with very little gas saturation is an appropriate simplification for this geothermal analysis. Since we have only one element in the vertical direction, we have selected a temperature of 300 °C as a typical for this reservoir. The pressure will be calculated by the equation of state to correspond to the small gas saturation. Having all cells in a two-phase state will also reduce the number of state transitions (two-phase to single-phase or single-phase to two-phase) that make convergence more difficult.

Edit Injection and Production Cells

The total injection/production from each five spot pattern is 30 kg/sec. Since we are using quarter symmetry, the production and injection mass flow rates will be 7.5 kg/sec. In this example we edit specific cells to specify injection and production parameters.

When editing individual cells, it is sometimes convenient to use the top view. To switch to the top view: in the **View** menu, click **Top View**.

To define the injection cell:

1. Right-click the lower left cell (ID=1), in the popup menu click **Edit Cells...**
2. In the **Cell Name** box, type *Injection*
3. Click the **Sources/Sinks** tab
4. Under **Injection**, select the **Water/Steam** check box
5. In the **Rate** box, type *7.5*
6. In the **Enthalpy** box, type *50000*

7. Click the **Print Options** tab
8. Click to select all time dependent output check boxes
9. Click **OK** to save changes and close the dialog

To define the production cell:

1. Right-click the upper right cell (ID=100), in the popup menu click **Edit Cells...**
2. In the **Cell Name** box, type *Production*
3. Click the **Sources/Sinks** tab
4. Under **Production**, select the **Mass Out** check box
5. In the **Rate** box, type *7.5*
6. Click the **Print Options** tab
7. Click to select both time dependent output check boxes
8. Click **OK** to save changes and close the dialog

The injection and production cells now appear in the tree at the left under the **Named/Print Cells** heading. Any cell that has been selected for time dependent output or explicitly named will appear in this list.

Edit Solution Controls

Parameters relating to the solver and time stepping can be found in the Solution Controls dialog.

To specify the simulation end time:

1. On the **Analysis** menu, click **Solution Controls**
2. In the **End Time** list, click **User Defined** and type *36.5 years*
3. Click **OK**

Edit Output Controls

By default, the simulation will print output every 100 time steps. For this simulation, we will specify output every 5 time steps.

To specify the output frequency:

1. On the **Analysis** menu, click **Output Controls**
2. In the **Print and Plot Every # Steps** box, type *5*
3. Click **OK**

Save and Run

The input is complete and you can run the simulation. The simulator will generate numerous output files (e.g. FOFT, mesh.csv, etc.). Since these files have the same name for every simulation, it is usually a good idea to create a folder specifically for a particular model.

To save your model:

1. On the **File** menu, click **Save**
2. Select a location, then click **Save**

To run the simulation:

1. On the **Analysis** menu, click **Run TOUGH2**

You should see a graph showing the increase in time step size as the simulation converges. If there are any problems, you can view the log. Output that has been identified as errors will appear in red.

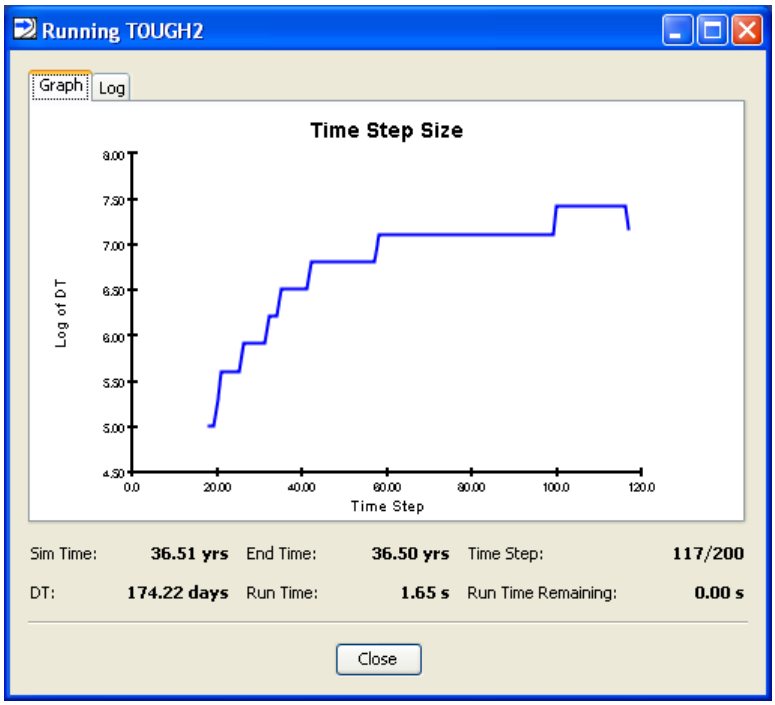

Figure 1.2: The Running TOUGH2 dialog shows a graph of time step size.

The **Simulation Complete** dialog will notify you when the end time has been reached. Click **OK** to dismiss the notification and click **Close** to exit the **Running TOUGH2** dialog.

View 3D Results

To open the **3D Results** dialog:

1. On the **Results** menu, click **3D Results**

By default, the display will show isosurfaces corresponding to pressure for the first output step.

To show temperature isosurfaces for the last time step:

1. In the **Scalar** list, click **T**
2. In the **Time(s)** list, click the last entry (t = **1.152E09**)

To show scalar data on a slice plane:

1. Click **Slice Planes...**
2. In the **Axis** list, click **Z**
3. In the **Coord** box, type *100*
4. Click **Close**

To remove isosurfaces and show only slice data:

1. Click to clear the **Show Isosurfaces** check box

The resulting visualization is shown below. Note the temperature drop at the production well. This is a result of specifying a production flow rate, which results in a lower pressure than would physically occur in a real well. This will be discussed further in the next example.

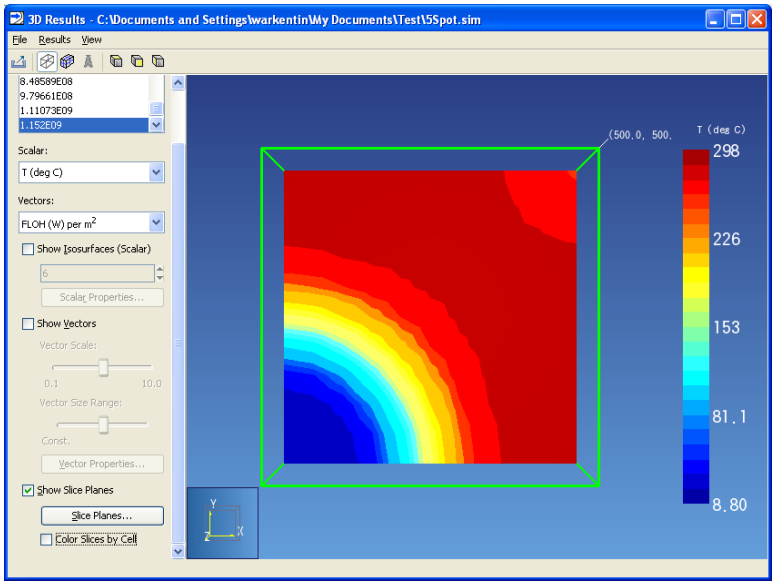

Figure 1.3: Temperature contours at end of solution

When finished, you can close the **3D Results** dialog.

View Time History Plots

To view time history plots:

1. On the PetraSim **Results** menu, click **Cell History Plots**
2. In the **Variable** list, click **T (deg C)**
3. In the **Cell Name** list, click **Injection**

The resulting plot is shown below.

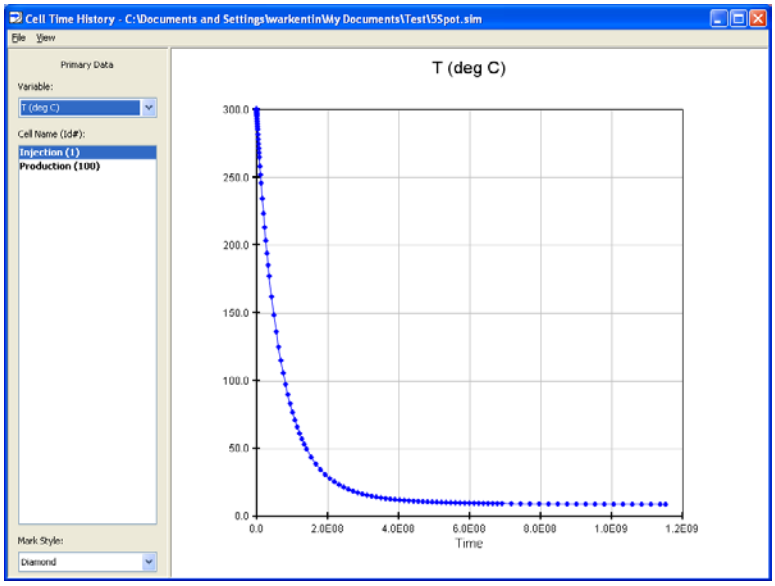

Figure 1.4: Temperature history of injection cell.

When finished, you can close the **Cell History** dialog.

2. Production from a Geothermal Reservoir (EWASG)

Description

This example is Problem 12 - Production from a Geothermal Reservoir with Hypersaline Brine and CO2 (EWASG) described in the TOUGH2 User's Manual (1). This problem examines production from a hypothetical geothermal reservoir with high salinity and CO2. Fluid withdrawal causes pressure to drop near the production well. Boiling of reservoir fluid gives rise to dilution of CO2 in the gas phase and to increased concentrations of dissolved NaCl, which begins to precipitate when the aqueous solubility limit is reached. As the boiling front receded from the well, solid precipitate fills approximately 10% of the original void space, causing permeability to decline to approximately 28% of its original value.

The mesh uses a 1D radial geometry.

Create an EWASG Model

We will first create a new model using the EWASG EOS.

From the **File** menu, select **New…** to open the **New Model** dialog.

1. For the **Simulator Mode**, choose **TOUGH2**.
2. For the **Equation of State (EOS)**, choose **EWASG**.
3. For the **Model Bounds**, enter the values from Table 2.1.

Table 2.1: Model boundary dimensions

Axis	Min (m)	Max (m)
X	5.0	1000.0
Y	0.0	1.0
Z	-500.0	0.0

Click **OK** to close the **New Model** dialog and create the model.

Specify the Solution Mesh

The solution mesh must be specified in two steps. First the Z divisions must be specified per layer. Then the mesh can be created using the **Create Mesh** dialog.

Specify Z Divisions

We must first specify one Z division for the default layer. To do so, we will open the **Edit Layers** dialog. On the **Model** menu, select **Edit Layers…**.

1. In the layers list in the left-hand pane, select the **Default** layer.
2. In the right-hand pane, select **Regular** for **Dz**.
3. In the **Cells** box, type *1*.
4. In the **Factor** box, type *1.0*.

Click **OK** to apply the changes and close the **Edit Layers** dialog.

Create the Mesh

We will now create the radial solution mesh using the **Create Mesh** dialog. To open the dialog, on the **Model** menu, select **Create Mesh…**.

1. For the **Mesh Type**, select **Radial**.
2. For the **Divisions**, select **Regular**.
3. In the **Radial Cells** box, type *100*.
4. In the **Factor** box, type *1.03705*.

Click **OK** to create the mesh.

We have selected Radial Mesh as the mesh type. This means that a 2D cylindrical RZ mesh will be created in which X corresponds to cylindrical R, Z corresponds to cylindrical Z, and the Y coordinate corresponds to cylindrical Theta (which is not used). 100 cells extend in the R direction, with an X Factor of 1.03705. This means that each cell is 1.03705 times the size of the previous cell in the R direction. These were chosen to give a first cell length of 2.0 m, which is the value used in the TOUGH2 example. See the PetraSim User Manual for instructions on how to calculate the appropriate factor.

The resulting mesh is displayed in Figure 2.1. Click the **Front View** button on the toolbar or rotate the model until the front is visible.

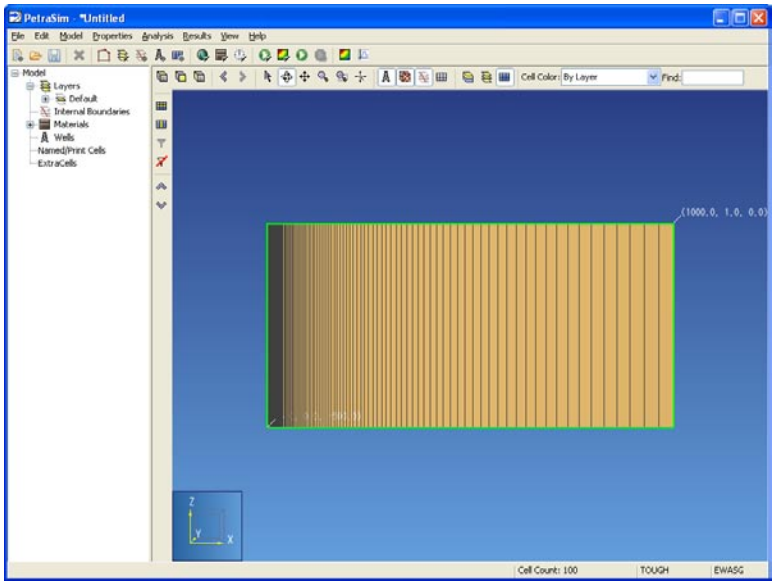

Figure 2.1: The resulting model

Global Properties

Global properties are those properties that apply to the entire model. We will make changes to some of the EOS options, including activating molecular diffusion. To edit global properties, you use the **Global Properties** dialog.

On the **Properties** menu, click **Global Properties…** (or click on the main toolbar).

1. In the **Global Properties** dialog, select the **Analysis** tab.
2. In the **Name** box, type *Geothermal Production, Brine and CO2*.
3. In the **Global Properties** dialog, select the **EOS** tab.
4. Select **Non-Isothermal**.
5. In the **Type of NCG** list, select **CO2**.
6. For **Dependence of Permeability on Pore Space**, select **Tubes in Series**.
7. In the **phi** box, type *0.8*.
8. In the **G** box, type *0.8*.
9. In the **Property Dependence on Salinity** list, select **Full Dependence**.
10. In the **Brine Enthalpy Correction** list, select **Michaelides**.
11. Select the **Include Vapor Pressure Lowering** checkbox.
12. Do NOT select **Molecular Diffusion**.
13. Click **OK** to close the **Global Properties** dialog.

Material Properties

To specify the material properties, use the **Material Data** dialog.

1. On the **Properties** menu, click **Edit Materials…** (or click on the toolbar).
2. In the **Name** box, type **POMED**.
3. In the **Density** box, type *2600.0*.
4. In the **Porosity** box, type *0.05*.
5. In all three **Permeability** boxes (X, Y, and Z), type *50e-15*.
6. In the **Wet Heat Conductivity** box, type *2.0*.
7. In the **Specific Heat** box, type *1000.0*.
8. Click **Apply** to save the changes.

In addition to the physical rock parameters, we also need to specify the relative permeability and capillary pressure functions for this material. These options can be found in the **Additional Material Data** dialog. To open this dialog, click the **Additional Material Data…** button.

To specify the relative permeability function

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **Corey's Curves**.
3. In the $\mathbf{S_{lr}}$ box, type *0.3*.
4. In the $\mathbf{S_{gr}}$ box, type *0.05*.

The default capillary pressure (none) is correct for this example.

Click **OK** to exit the **Advanced Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

The initial state of each cell in the model must be defined. To specify global initial conditions that will be used as the default for all cells in the model, on the **Properties** menu, click **Initial Conditions...** (or click on the toolbar).

To set the initial conditions

1. Select the **Two Fluid Phases (P, Xsm, Sg, T)** state option.
2. In the **Pressure** box, type *6.0E6*.
3. In the **Temperature** box, type *275.55*.
4. In the **Gas Saturation** box, type *0.45*.
5. In the **Salt Mass Fraction** box, type *0.3*.

Click **OK** to close the **Default Initial Conditions** dialog.

Define Reservoir Production

In this model, fluid is produced from the inner cell.

1. In the **3D View**, click the **Front View** button on the toolbar or rotate the model until the front is visible.
2. Use the **Zoom Box** tool to zoom in on the left side of the model until the left-most cell is visible.
3. Using the **3D Orbit Navigation** tool, right click the left-most cell and from the context menu, select **Edit Cells...** as shown in Figure 2.2.
4. In the **Cell Name** box, type *Production*.
5. Click the **Sources/Sinks** tab.
6. In the **Production** section, select the **Mass Out** check box.
7. In the **Rate** box, type *65*.
8. Click the **Print Options** tab.
9. Select the **Print Time Dependent Flow and Generation (BC) Data**.
10. Click **OK** to close the **Edit Cell Data** dialog.

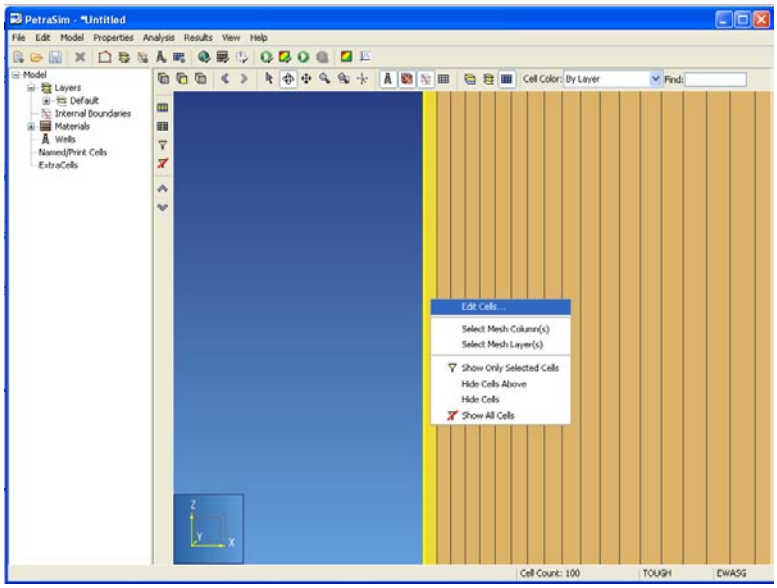

Figure 2.2: The cell to be selected

Solution Controls

We will now define the solution control options.

1. On the **Analysis** menu, click **Solution Controls…** (or click on the main toolbar).
2. In the **End Time** box, type *2.0E6* (approximately 23 days).
3. In the **Time Step** list, ensure that *Single Value* is selected.
4. In the **Time Step** box, type *1000*. This is the initial time step.
5. Select **Enable Automatic Time Step Adjustment**.
6. Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, the simulation will print output every 100 time steps. We can increase the frequency of the output in the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls…** (or click on the main toolbar).
2. In the **Print and Plot Every # Steps** box, type *10*.
3. Next to the **Additional Print & Plot Times**, click the **Edit…** button.
4. In the **Additional Print Times** table, type *.50E5*. This will force a solution printout at this time.
5. Click **OK** to exit the **Additional Print Times** dialog.
6. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can run the simulation. If you haven't already, you may want to save your model in a new directory. For example

1. On the **File** menu, click **Save** (or click on the main toolbar).

2. Create a new folder named *ewasg_geothermal* and in the **File Name** box, type *geothermal.sim*.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2** (or click on the main toolbar).

During the solution, a graph will display the time step size.

View 3D Results

To view the 3D results for a simulation, on the **Results** menu, click **3D Results** (or click on the main toolbar). The data for the current simulation will be automatically loaded and displayed.

To show gas saturation contours for the last time step

1. In the **Time(s)** list, select the last entry (**2.0E6**).
2. In the **Scalar** list, select **SG**.
3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes…**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Y**.
2. In the **Coord** box, type *0.5*.
3. Select the **Scalar** check box.
4. Click **Close**.

To orient and view the model with mesh

1. Click the **Front View** button on the toolbar or rotate the model until the front is visible.
2. On the **View** menu, click **Show Mesh**.

The view can be zoomed and panned by holding the Alt and Shift keys, respectively, and dragging the mouse. After moving the view to the upper left corner of the model, the resulting contour plot is shown in Figure 2.3.

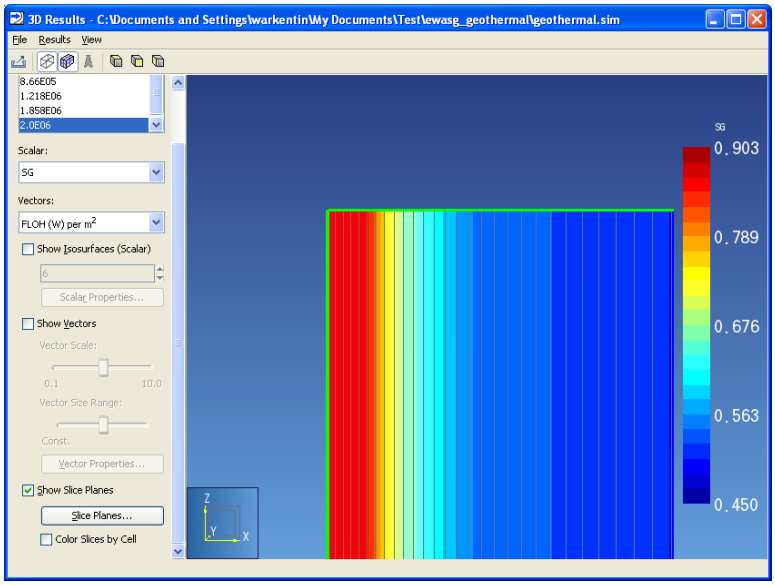

Figure 2.3: 3D representation of the saturation of gas

Close the **3D Results** window.

View Cell History Plots

You can view time history plots with the **Cell History** dialog. On the **Results** menu, click **Cell History Plots** (or click on the main toolbar).

The **Cell History** dialog will be displayed. In this window, you can display time history data using a plotting parameter and a list of cells. For example, to view the gas saturation in the Heat Source cell

1. In the **Variable** list, select **SG**.
2. In the **Cell Name** list, select **Production**.

Figure 2.4 shows the time history plot of SG at the production cell. The user can export this data for plotting in spreadsheets.

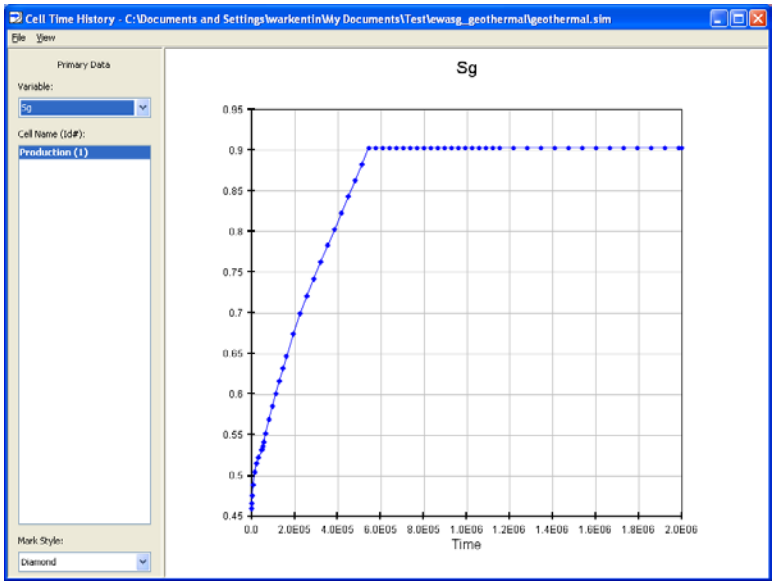

Figure 2.4: The cell history plot for gas saturation in the production cell

Close the **Cell History** window.

Line Plots

PetraSim also supports line plots, where you define a line in 3D space and the data is interpolated along the line. To make a line plot

1. First open the 3D results view. On the **Results** menu, click **3D Results** (or click on the main toolbar).
2. On the **File** menu, click **Line Plot…**.
3. In the **Point 1** coordinate boxes (**X, Y,** and **Z**) type *5.0, 0.5,* and *-250.0*, respectively.
4. In the **Point 2** coordinate boxes (**X, Y,** and **Z**) type *1000.0, 0.5,* and *-250.0*.
5. Click **OK** to close the **Line Plot** dialog.
6. This will open a **Line Plot** window.
7. In the **Variable** list, select **P (Pa)**.
8. In the **Time** list, select **2.0E06** (the last time).

The plot is shown in Figure 2.5. You can export this data to a comma separated value file for import into a spreadsheet.

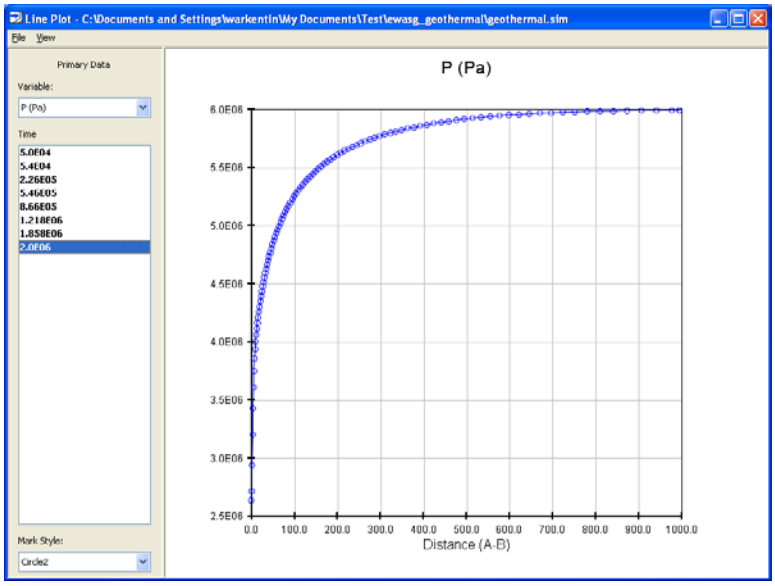

Figure 2.5: Line plot of pressure

Close the **Line Plot** window.

Data saved using the line plot are shown in the same format as in the TOUGH2 user's manual in Figure 2.6. The calculated results compare well with the manual results.

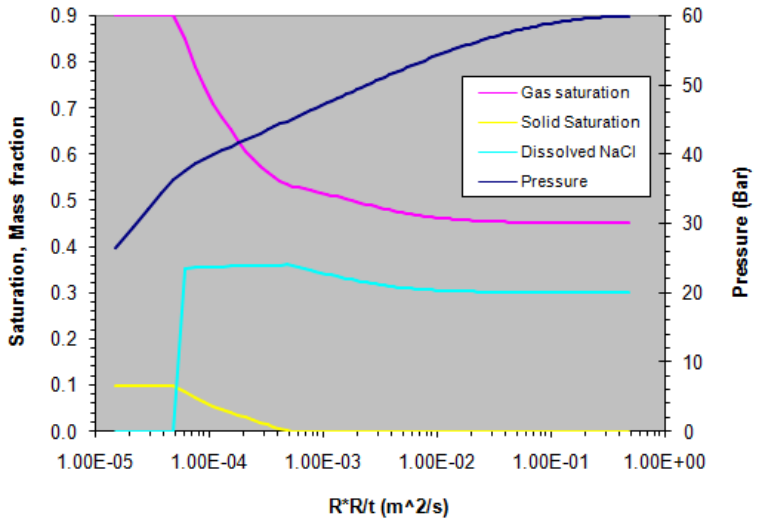

Figure 2.6: Results for comparison with TOUGH2 manual

3. 2D Steam Replacement (T2VOC)

Description

This example demonstrates one dimensional gas diffusion of an organic chemical with phase partitioning - as described in the T2VOC User's Guide (2).

A horizontal column has an initial temperature of 10° C and an initial pressure of 101325 Pa. The left cell has a fixed thermodynamic state and acts as a source of chlorobenzene. The geometry of the problem is shown in Figure 3.1.

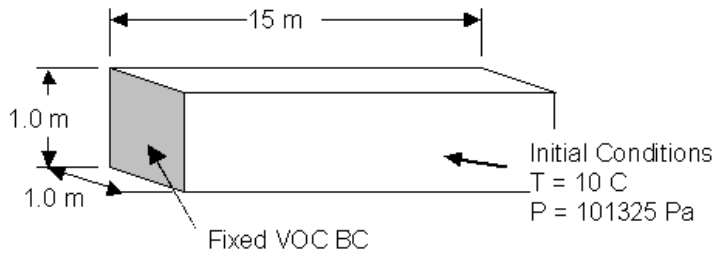

Figure 3.1: Example Problem Overview

We will use a mesh with 150 cells in the horizontal direction.

Create a T2VOC Model

We will first create a new model using the T2VOC EOS.

From the **File** menu, select **New…** to open the **New Model** dialog.

1. For the **Simulator Mode**, choose **TOUGH2**.
2. For the **Equation of State (EOS)**, choose **T2VOC**.
3. For the **Model Bounds**, enter the values from Table 2.1.

Table 3.1: Model boundary dimensions

Axis	Min (m)	Max (m)
X	0.0	15.0
Y	0.0	1.0
Z	0.0	1.0

Click **OK** to close the **New Model** dialog and create the model.

You can rotate, pan, and zoom the model using the mouse and **Shift** and **Alt** keys. The resulting boundary is shown in Figure 3.2. PetraSim will automatically add labels for the min point and max point of the boundary.

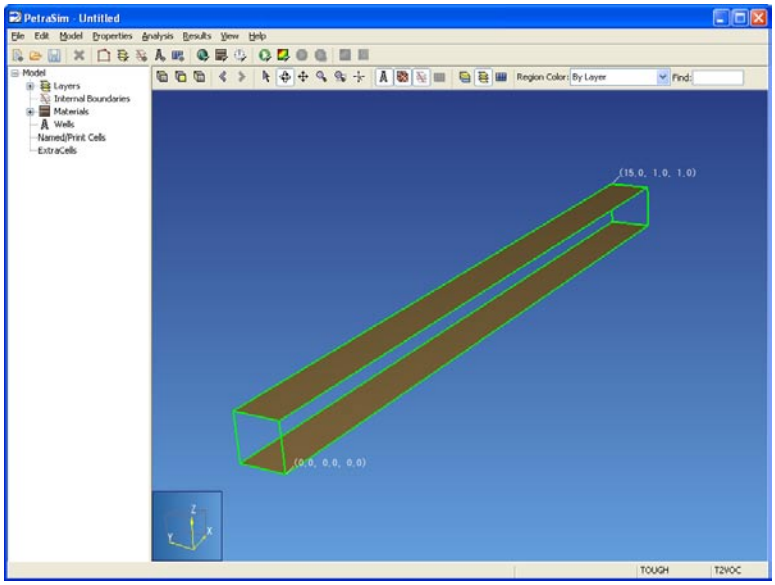

Figure 3.2: The Model Boundary

Specify the Solution Mesh

The solution mesh must be specified in two steps. First the Z divisions must be specified per layer. Then the mesh can be created using the **Create Mesh** dialog.

Specify Z Divisions

We must first specify one Z division for the default layer. To do so, we will open the **Edit Layers** dialog. On the **Model** menu, select **Edit Layers…**.

1. In the layers list in the left-hand pane, select the **Default** layer.
2. In the right-hand pane, select **Regular** for **Dz**.
3. In the **Cells** box, type *1*.
4. In the **Factor** box, type *1.0*.

Click **OK** to apply the changes and close the **Edit Layers** dialog.

Create the Mesh

We will now create the radial solution mesh using the **Create Mesh** dialog. To open the dialog, on the **Model** menu, select **Create Mesh…**.

1. For the **Mesh Type**, select **Regular**.
2. For the **Divisions**, select **Regular**.
3. In the **X Cells** box, type *150*.
4. In the **Y Cells** box, type *1*.
5. For both **X** and **Y Factor**s, type *1.0*.

Click **OK** to create the mesh.

Global Properties

Global properties are those properties that apply to the entire model. In this example we will set the simulation name and configure the simulation VOC. To edit global properties, you can use the **Global Properties** dialog.

On the **Properties** menu, select **Global Properties…**.

Simulation Name

1. In the **Global Properties** dialog, select the **Analysis** tab.
2. In the **Name** box, type *T2VOC Problem 1*.

EOS Data

The EOS (Equation of State) tab displays options for the T2VOC simulator. In this example, we will perform an isothermal (no heat flow) analysis. We will also specify a variant of chlorobenzene as the simulation VOC and specify the Air-Vapor diffusion constant.

In the **Global Properties** dialog, select the **EOS** tab.

By default, the simulator will run in isothermal mode. Nothing needs to be changed.

To specify the VOC, you will need to create a variant of chlorobenzene using the **Edit VOC Data** dialog.

1. Click **Edit VOC Data…**.
2. Click **New**.
3. In the **Name** box, type *Chlorobenzene Ex 1*.
4. In the **Based On** list, select **Chlorobenzene (STD)**.
5. Click **OK**. This creates a new VOC.
6. Update the values for **CHEMP.4**, **CHEMP.6**, and **CHEMP.7** according to the values shown in Table 3.2, Table 3.3, and Table 3.4.
7. Click **OK** and ensure that the selected **Simulation VOC** is **Chlorobenzene Ex 1**.
8. This simulation will use gas diffusion. You can enable gas diffusion by setting the **Air-Vapor Diffusion** to a non-zero value. In the **Air-Vapor Diffusion** box, type *2.13e-5*.
9. Click **OK** to close the **Global Properties** dialog.

Table 3.2: Chlorobenzene Ex 1 (CHEMP.4)

Field	Value
Reference Density for NAPL	1106.0
Reference Temperature for NAPL	293
Reference Binary Diffusivity of VOC in Air	8.0e-6
Reference Temperature for Gas Diffusivity	283.15
Chemical Diffusivity Exponent	1.0

Table 3.3: Chlorobenzene Ex 1 (CHEMP.6)

Field	Value
SOLA	7.99e-5
SOLB	0.0
SOLC	0.0
SOLD	0.0

Table 3.4: Chlorobenzene Ex 1 (CHEMP.7)

Field	Value
Chemical Organic Carbon Partition Coef	0.15
Default Fraction of Organic Carbon in Soil	0.005
VOC Biodegradation Decay Constant	0.0

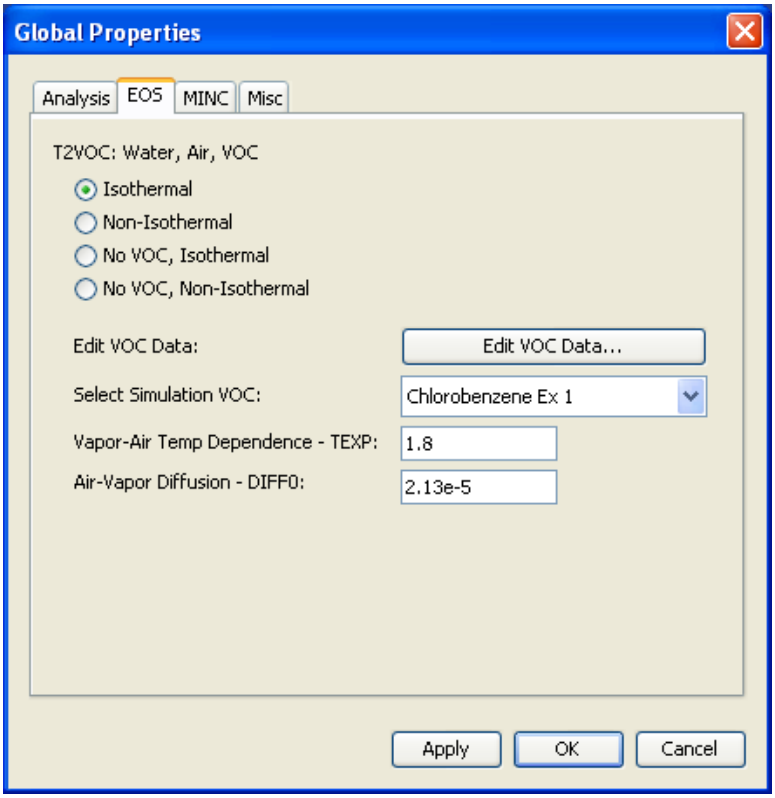

Figure 3.3: T2VOC Simulation Parameters

Material Properties

To specify the material properties, you can use the **Material Data** dialog.

1. On the **Properties** menu, click **Edit Materials…**.
2. In the **Name** box, type *DIRT1*.
3. In the **Density** box, type *2650.0*.

4. In the **Porosity** box, type *0.4*.
5. In all three **Permeability** boxes, type *1e-14*.
6. In the **Wet Heat Conductivity** box, type *3.1*.
7. In the **Specific Heat** box, type *1000.0*.
8. Click **Apply** to save the changes.

We still need to specify the relative permeability function and fraction of organic carbon for this material. These options can be found in the **Advanced Material Data** dialog. To open this dialog, click the **Additional Material Data…** button.

To specify the relative permeability function:

1. Select the **Relative Perm** tab.
2. In the **Relative Permeability** list, select **Stone's 3-Phase**.
3. In the $\mathbf{S_{wr}}$ box, type *0.4*.
4. In the $\mathbf{S_{nr}}$ box, type *0.1*.
5. In the $\mathbf{S_{gr}}$ box, type *1.0e-3*.
6. In the **n** box, type *1.0*.

The default capillary pressure (none) is correct for this example.

To specify the fraction of organic carbon:

1. Select the **Misc** tab.
2. In the **Fraction of Organic Carbon** box, type *0.005*.

Click **OK** to exit the **Additional Material Data** dialog.

Click **OK** again to save your settings and exit the **Material Data** dialog.

Initial Conditions

You can control the initial state of the primary variables using initial conditions. Primary variable selection will depend on several factors including EOS selection, simulator mode, and the initial state of the simulation. You can edit initial conditions globally and on a cell-by-cell basis.

To edit global initial conditions: on the **Properties** menu, select **Initial Conditions…**.

For this example, we will initialize all cells to a two-phase water and air state. There is no initial chlorobenzene saturation. To set the initial conditions:

1. Select the **Two-Phase Water/Air** state option.
2. In the **Pressure** box, type *101325.0*.
3. In the **Temperature** box, type *10.0*.
4. In the **Water Saturation** box, type *0.25*.
5. In the **VOC Mole Fraction in Air** box, type *0.0*.
6. Click **OK**.

Boundary Conditions

We will inject chlorobenzene into the model using a cell-specific initial condition. Then we will force the state of that cell to remain constant. To edit individual cells, you can use the **3D View**.

Every cell in the model has a unique ID number. You can find and select cells based on their ID number using the **Find** field in the upper-right corner of the **3D View**. In this example, cell 1 will be the chlorobenzene source. To find and select cell 1:

1. In the **Find** box, type *1*.
2. Press *ENTER*. The cell should be selected and shown in the center of the **3D View**.

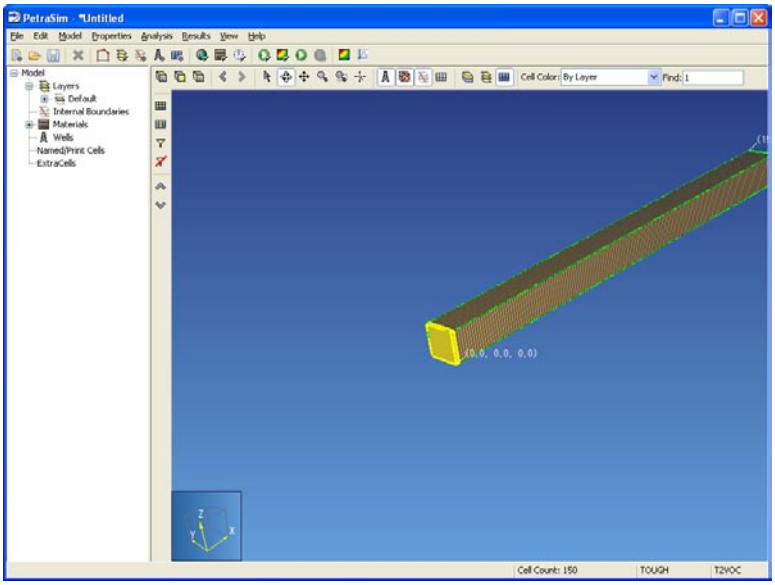

Figure 3.4: Finding a Cell in the 3D View

You can now edit the properties of cell 1. Ensure cell 1 is selected. On the **Edit** menu, select **Properties…**.

To force the state of this cell to remain constant throughout the simulation, you can adjust its type. Select the **Properties** tab. Then, in the **Type** list, select **Fixed State**.

Now you can give the cell a custom initial condition that will remain constant throughout the simulation. Select the **Initial Conditions** tab. To enter the custom initial conditions:

1. Select **Specify Initial Conditions by Cell**.
2. Select the **Three-Phase Water/Air/NAPL** state.
3. In the **Gas Saturation** box, type *0.75*.
4. In the **Water Saturation** box, type *0.2*.

Notice that we did not explicitly specify a NAPL saturation. With the gas saturation at *0.75* and the water saturation at *0.2* the NAPL saturation will be *0.05*. T2VOC will perform this calculation during the simulation.

Click **OK** to close the **Edit Cell Data** dialog.

Solution Controls

We will now adjust the time step T2VOC will use while executing the simulation. Options relating the time step and other simulation options can be found in the **Solution Controls** dialog.

To open the **Solution Controls** dialog: on the **Analysis** menu, click **Solution Controls…**.

For this example, we will adjust the end time, increase the maximum number of time steps, and limit the size of the maximum time step.

1. In the **End Time** box, type *1 yr*.
2. In the **Max Num Time Steps** box, type *350*.
3. In the **Max Time Step** list, select **User Defined**.
4. In the **Max Time Step** box, type *5 days*.

Click **OK** to exit the **Solution Controls** dialog.

Output Controls

By default, T2VOC will print output every 100 time steps. We can increase the resolution of the output with the **Output Controls** dialog.

1. On the **Analysis** menu, click **Output Controls…**.
2. In the **Print and Plot Every # Steps** box, type *5*.
3. Click **OK** to exit the **Output Controls** dialog.

Save and Run

The input is complete and you can now run the simulation. Bear in mind that T2VOC generates many output files and they will overwrite the output from any previous simulations in a directory. If you haven't already, you may want to save your model in a directory specifically intended for the simulation results. For example:

1. On the **File** menu, click **Save**.
2. Create a new folder named *t2voc_problem_1* and in the **File Name** box, type *t2voc_prob1.sim*.
3. Click **Save**.

To run the simulation, on the **Analysis** menu, click **Run TOUGH2**.

During the solution, a graph will display the time step size. In this case, the time steps increase until they remain constant at the specified maximum.

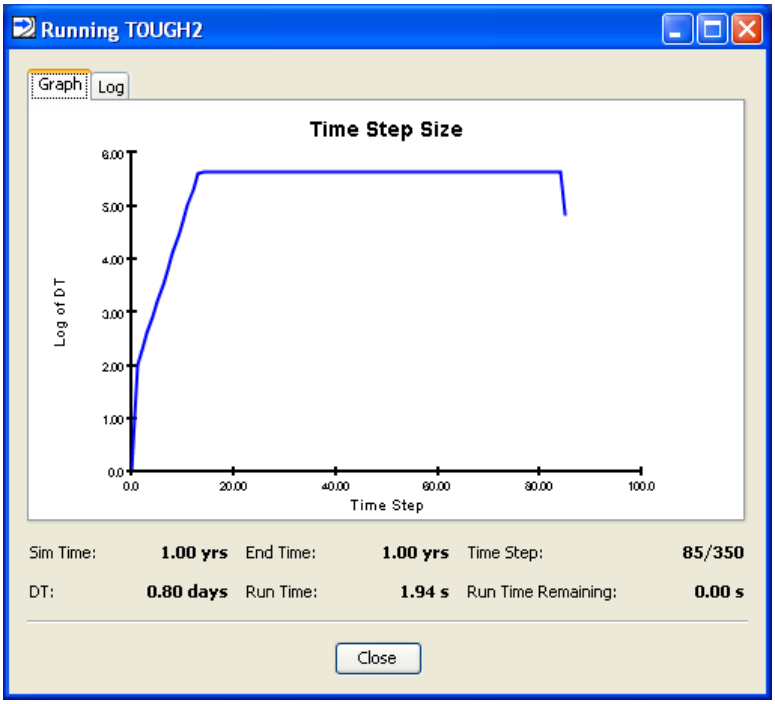

Figure 3.5: Running T2VOC

View 3D Results

To view the 3D results for a simulation

1. On the **Results** menu, click **3D Results**. The data for the current simulation will be automatically loaded and displayed.

To view the VOC concentration for the last time step.

1. In the **Time(s)** list, select the last entry (**3.156E07**).
2. In the **Scalar** list, select **CVOCGAS**.
3. Click to clear the **Show Isosurfaces** checkbox.

To add a slice plane on which contours will be displayed, click **Slice Planes…**. For this example we will show one slice plane. To configure the slice plane

1. In the **Axis** list, select **Z**.
2. In the **Coord** box, type *0.5*.
3. Ensure that the **Scalar** check box is checked.
4. Click **Close**.

Your results should now look similar to the screenshot in Figure 3.6. You can now see the gas-phase VOC concentration emanating from the left side of the model.

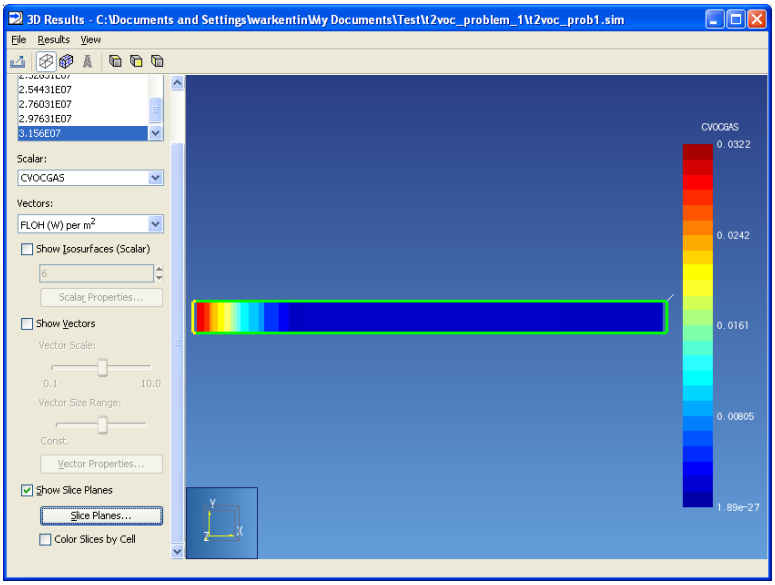

Figure 3.6: T2VOC 3D Results

Close the **3D Results** window.

References

1. **Pruess, Karsten, Oldenburg, Curt and Moridis, George.** *TOUGH2 User's Guide, Version 2.0.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, November 1999. LBNL-43134.

2. **Falta, Ronald, et al.** *T2VOC User's Guide.* Berkeley, CA, USA : Earth Sciences Division, Lawrence Berkeley National Laboratory, March 1995. LBNL-36400.